

Energy functional based on natural orbitals and occupancies for static properties of nuclei.

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Abstract. The possibility to use functionals of occupation numbers and natural orbitals for interacting fermions is discussed as an alternative to multi-reference energy density functional method. An illustration based on the two-level Lipkin model is discussed.

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INTRODUCTION

The nuclear many-body problem of N interacting nucleons can be solved exactly only in very specific cases or for very small particle numbers. This is due to the large number of degrees of freedom involved in such a complex system. Let us for instance consider particles interacting through a Hamiltonian written as

$$H = \sum_{ij} t_{ij} a_i^+ a_j + \frac{1}{4} \sum_{ijkl} \tilde{v}_{ijkl} a_i^+ a_j^+ a_l a_k + \dots \quad (1)$$

Then the exact ground state energy can be written as

$$E_{\text{Exact}}(\gamma^{(1)}, \gamma^{(2)}, \dots) = \sum_{ij} t_{ij} \gamma_{ji}^{(1)} + \frac{1}{4} \sum_{ijkl} \tilde{v}_{ijkl} \gamma_{kl,ij}^{(2)} + \dots, \quad (2)$$

where $\gamma_{ji}^{(1)} \equiv \langle a_i^+ a_j \rangle$, $\gamma_{kl,ij}^{(2)} \equiv \langle a_i^+ a_j^+ a_l a_k \rangle$, ... denote the one-, two-, ... body density matrices that contain all the information on the one-, two-...body degrees of freedom respectively. A natural way to reduce the complexity of this problem is to assume that at a given level, the k -body (and higher-order) density matrices becomes a functional of the lower-order ones. This is what is done for instance in the Hartree-Fock (HF) approximation where all k -body density matrices (with $k \geq 2$) become a functional of $\gamma^{(1)}$. Unfortunately, the HF theory applied to the nuclear many-body problem in terms of the vacuum Hamiltonian is a poor approximation and Many-Body theories beyond HF are necessary.

The introduction of Energy Density Functional (EDF) approaches in the 70's was a major breakthrough (see for instance [1] for a recent review). In its simplest form, the EDF formalism starts with an energy postulated as a functional of $\gamma^{(1)}$, the latter being built out of a Slater Determinant. Then the ground state energy is obtained by minimizing

the energy with respect to $\gamma^{(1)}$, i.e.

$$E_{\text{Exact}} \simeq \mathcal{E}_{\text{MF}}(\gamma^{(1)}) \quad (3)$$

Parameters are generally adjusted on specific experimental observations and therefore encompass directly many-body correlations. Current EDF uses a generalization of eq. (3) obtained by considering quasi-particle vacua as trial states. By making explicit use of symmetry breaking, such a functional called hereafter Single-Reference (SR-) EDF is able to account for static correlation associated with pairing and deformation. Actual SR-EDF takes the form ¹:

$$E_{\text{Exact}} \simeq \mathcal{E}_{\text{MF}}(\gamma^{(1)}) + \mathcal{E}_{\text{Cor}}(\kappa, \kappa^*) \quad (4)$$

where κ denotes the anomalous density. To restore symmetries and/or incorporate dynamical correlations, guided by the Generator Coordinate Method (GCM), a second level of EDF implementation, namely Multi-Reference (MR-) EDF is introduced. Recently, difficulties with the formulation and implementation of have been encountered in MR-EDF. A minimal solution has been proposed in ref. [2, 3, 4]. Besides these problems, the authors of ref. [2] have pointed out the absence of a rigorous theoretical framework for the MR EDF approach. At the heart of the problem is the possibility to break symmetries in functional theories and then restore them using configuration mixing. This issue needs to be thoroughly addressed in the future.

In this context, it is interesting to see if extensions of the functional used at the SR-EDF level can grasp part of the effects that for standard functionals require the MR level. It is worth realizing that, in the canonical basis for which $\gamma^{(1)} = \sum_i |\varphi_i\rangle n_i \langle \varphi_i|$, we have

$$\mathcal{E}_{\text{Cor}}(\kappa, \kappa^*) = \mathcal{E}_{\text{Cor}}[\{\varphi_i, n_i\}] = \frac{1}{4} \sum_{i,j} \bar{v}_{ii\bar{j}\bar{j}}^{\kappa\kappa} \sqrt{n_i(1-n_i)} \sqrt{n_j(1-n_j)}, \quad (5)$$

and therefore, the energy can be regarded as a functional of natural orbitals φ_i and occupation numbers n_i . As a matter of fact, for electronic systems, Gilbert has generalized the Kohn-Sham theory and shown that the exact energy of a system can be obtained by minimizing such a functional [5] leading to the so-called Density Matrix Functional Theory (DMFT). The possibility to consider occupation numbers as building blocks of the nuclear energy functional has recently been discussed in ref. [6, 7]. Two levels of theory can be developed along the line of Gilbert's idea (i) either, functionals in the strict Gilbert framework can be designed. In that case, since the density identify with the exact density at the minimum, it should respect all symmetries of the bare Hamiltonian. (ii) or we exploit the concept of symmetry breaking. In the latter case, similarly to the SR-EDF, strictly speaking we cannot anymore rely on the theorem, but we may gain better physical insight with relatively simple functionals.

¹ Note that the denomination "mean-field" or the separation into a "mean-field" like and "correlation" like is completely arbitrary since, as we mention previously, the so-called "mean-field" part already contains correlation much beyond a pure Hartree-Fock approach.

APPLICATION TO THE LIPKIN MODEL AND DISCUSSION

The descriptive power of DMFT is illustrated here in the two-level Lipkin model [10]. In this model, the Hartree-Fock (HF) theory fails to reproduce the ground state energy whereas configuration mixing like Generator Coordinate Method (GCM) provides a suitable tool [8, 9]. Therefore, the two-level Lipkin model is perfectly suited both to illustrate that DMFT could be a valuable tool and to provide an example of a functional for system with a "shape" like phase-transition. In this model, one considers N particles distributed in two N -fold degenerated shells separated by an energy ε . The associated Hamiltonian is given by $H = \varepsilon J_0 - \frac{V}{2}(J_+ J_+ + J_- J_-)$ where V denotes the interaction strength while J_0, J_{\pm} are the quasi-spin operators defined as $J_0 = \frac{1}{2} \sum_{p=1}^N (c_{+,p}^\dagger c_{+,p} - c_{-,p}^\dagger c_{-,p})$, $J_+ = \sum_{p=1}^N c_{+,p}^\dagger c_{-,p}$ and $J_- = J_+^\dagger$. $c_{\pm,p}^\dagger$ and $c_{\pm,p}$ are creation operators associated with the upper and lower levels respectively. Due to the specific form of the Lipkin Hamiltonian, $\gamma^{(1)}$ simply writes in the natural basis as $\gamma^{(1)} = \sum_{p=1}^N \left\{ |\varphi_{0,p}\rangle n_0 \langle \varphi_{0,p}| + |\varphi_{1,p}\rangle n_1 \langle \varphi_{1,p}| \right\}$ with $n_1 = (1 - n_0)$. Introducing the angle α between the state $|-, p\rangle$ and $|\varphi_{0,p}\rangle$, leads to the following mean-field functional [11]

$$\mathcal{E}_{\text{MF}}(\{\varphi_{i,p}, n_i\}) = \mathcal{E}_{\text{MF}}(\alpha, n_0) = -\frac{\varepsilon}{2} N \left\{ \cos(2\alpha)(2n_0 - 1) + \frac{\chi}{2} \sin^2(2\alpha)(2n_0 - 1)^2 \right\}. \quad (6)$$

where $\chi = V(N - 1)/\varepsilon$. This expression is easily obtained by generalizing the Hartree-Fock case (recovered here if $n_0 = 1$). The main challenge of the method is to obtain an accurate expression for \mathcal{E}_{Cor} . To get the functional, clearly identified cases from which properties of the functional could be inferred have been used[11], namely the $N = 2$ case and the large N limit. In the two-particles case, the correlation energy can be analytically obtained and reads

$$\mathcal{E}_{\text{Cor}}^{N=2}(\alpha, n_0) = -2V \left\{ \sin^2(2\alpha)n_0(1 - n_0) + (\sin^4(\alpha) + \cos^4(\alpha)) \sqrt{n_0(1 - n_0)} \right\} \quad (7)$$

A simple extension of the $N = 2$ case for larger number of particles is to assume that each pair contributes independently from the others leading to $\mathcal{E}_{\text{Cor}}^N = [N(N - 1)/2] \mathcal{E}_{\text{Cor}}^{N=2}$. However, such a simple assumption leads to a wrong scaling behavior in the large N limit. Indeed, in this case, $\mathcal{E}_{\text{Cor}}^N \propto N^2$ as N tends to infinity while a $N^{4/3}$ scaling is expected [12]. To obtain the correct limit, a semi-empirical factor $\eta(N)$ can be introduced such that

$$\mathcal{E}_{\text{Cor}}^{N \geq 3}(\alpha, n_0) = \eta(N) \frac{N(N - 1)}{2} \mathcal{E}_{\text{Cor}}^{N=2}(\alpha, n_0), \quad (8)$$

with $\eta(N) = cN^{-2/3}$. The value $c = 1.5$ has been retained using a fitting procedure. Examples of results obtained by minimizing the functional given by Eqs. (6) and (8) are shown in Fig. 1 for different particle numbers and interaction strengths. In all cases, a very good agreement, much better than the HF case is found.

The Lipkin example suggests that DMFT can be a valuable tool for describing ground state of a many-body system when symmetry breaking plays a significant role. The

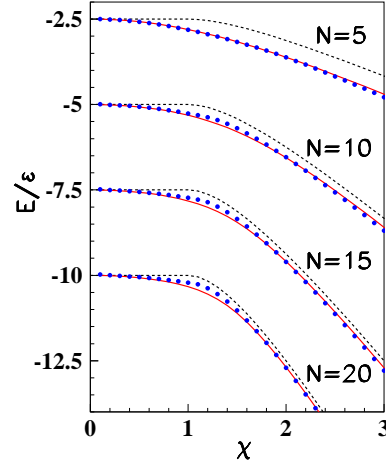


FIGURE 1. Exact ground state energy (solid lines) displayed as a function of χ for $N = 5$ to 20 resp. from top to bottom. In each case, the corresponding HF (dashed line) and DMFT (filled circle) minimum energy are shown. The DMFT calculation is performed using the mean-field and correlation energy resp. given by Eq. (6) and Eq. (8) with $\eta(N) = 1.5 N^{-2/3}$ (Adapted from [11]).

functional designed here is exact only in the $N = 2$. Note that the functional proposed here breaks signature symmetry and therefore enters into the level (ii) of functional discussed in the introduction. The Lipkin model is however rather schematic and cannot be used as a guidance for realistic situations. The possibility to design a new accurate functional for nuclei remains a challenging problem.

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